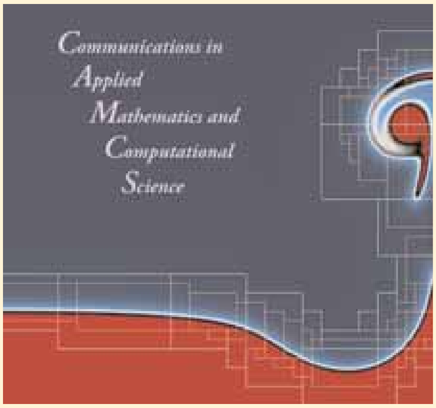
CRD report

News from the LBNL Computational Research Division July 2005



CRD Mathematicians Help Launch New Math Journal

Four LBNL mathematicians — John Bell, Phil Colella, Alexandre Chorin and James Sethian — are members of the editorial team which has launched Communications in Applied Mathematics and Computational Science (CAMCoS). Other editors are Marsha Berger and Leslie Greengard of the Courant Institute, Rupert Klein of the Freie Universitaet Berlin, and Raz Kupferman of the Hebrew University. Bell, who is head of CRD's Center for Computational Sciences and Engineering, is managing editor.

According to the CAMCoS Web site, "The Communications will publish high-quality original contributions to applied mathematics and computational science, with an emphasis on work where both the mathematics and the algorithms are of interest and where the mathematical outlook is at least partially new.

"The fields covered include the solution of ordinary, partial and stochastic differential equations; integral equations; numerical and analytical methods for fluid dynamics, biology, quantum and statistical mechanics; multiscale and underresolved problems; computational probability and Monte-Carlo methods. The emphasis in papers should be on methods and tools rather than on the specific physical conclusions in special cases."

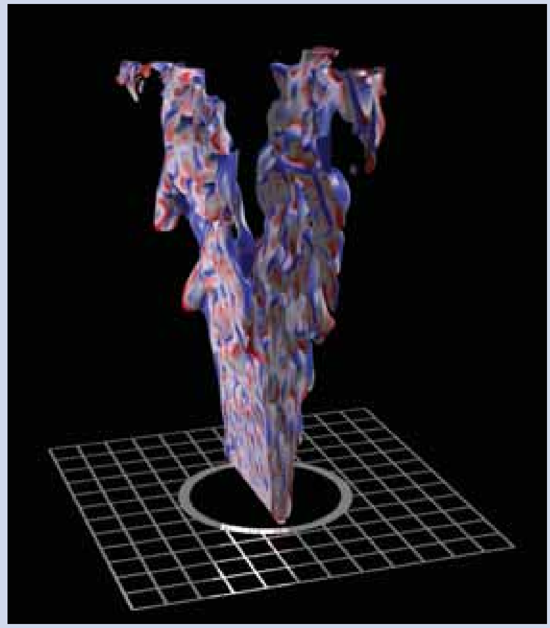
For more information about CAMCoS, go to <http://www.camcos.org>.

Groundbreaking Combustion Research by CRD Featured on Cover of Proceedings of National Academy of Sciences

Computational and combustion scientists at Berkeley Lab have earned national recognition in the July 19, 2005 Proceedings of the National Academy of Sciences with their cover article about unparalleled computer simulations of turbulent flames.

The research by scientists in CRD's Center for Computational Sciences and Engineering and in the Environmental Energy Technologies Division has led to a three-dimensional combustion simulation of unmatched size without resorting to models for turbulence or turbulence-chemistry interactions. The article shows that the simulation closely matches a combustion experiment.

Gaining a better understanding of combustion, which powers everything from automobiles to aircraft to power generating plants, can help improve the efficiency of those system as well as help reduce the amount of pollution produced by burning fossil fuels.



CCSE staff produced this 3D laboratory-scale turbulent flame simulation which closely matched a combustion experiment.

(continued on page 2)

DOE JGI Releases Latest Version of IMG

An enhanced version of the Integrated Microbial Genomes (IMG) data management system has been released by the U.S. Department of Energy (DOE) Joint Genome Institute (JGI). IMG 1.1 contains 32 new public genomes and 14 new genomes sequenced by DOE JGI, bringing the total of genomes in IMG to 337. These include 301 bacterial, 25 archaeal, and 11 eukaryotic genomes, of which 36 finished and 75 draft genomes were sequenced by DOE JGI.

The new IMG 1.1 features enhanced capabilities to improve the efficiency of the genome analysis process. To extend the utility of the organism and gene analysis tools, several new features have been added. These include a function to compare gene occurrence profiles across organisms, an enhanced support infrastructure for comparative organism statistics, and the ability to save and load organism and gene analysis settings from local user files. The documentation has been also expanded to ease the overall comprehensibility of IMG analysis.

IMG, accessible to the public at <http://img.jgi.doe.gov/>, is the result of a collaboration between the DOE JGI and the Lawrence Berkeley National Laboratory Biological Data Management and Technology Center (BDMTC). IMG continues to be updated on a quarterly basis with new public and DOE JGI genomes. The next update is scheduled for September 1, 2005.

CRD's Michael Wehner Gives Presentation at Climate Workshop

Michael Wehner of CRD's Scientific Computing Group was selected to give a presentation at a meeting of the Climate Change Working Group at the Tenth Annual CCSM Workshop held June 21–23 in Breckenridge, Colo.

The workshop is held annually for the Community Climate System Model (CCSM) project, which has been developed under the NSF's and DOE's sponsorship at NCAR, with the National Oceanic and Atmospheric Administration (NOAA), and the National Aeronautics and Space Administration (NASA) as part of the U.S. Global Change Research Program and the U.S. Climate Change Science Program. This year's workshop theme was "Crosscutting Science Using CCSM."

Wehner's talk was on "Changes in Daily Surface Air Temperature and Precipitation Extremes in the IPCC AR4." Last year, Wehner received an NSF grant to characterize the ability of coupled climate models to simulate extreme weather events. The ability of these models to accurately simulate historical climate changes in the twentieth century will determine the credibility of their predictions of climate change during the twenty-first century and beyond.

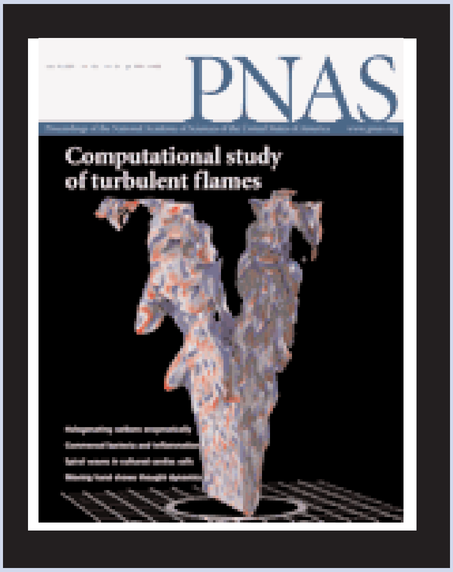
Wehner's grant was funded as part of the U.S. Climate Variability and Predictability (CLIVAR) project. A report summarizing aspects of this work will be furnished to the lead authors of the relevant chapters for the Intergovernmental Panel on Climate Change's Assessment Report Four (IPCC AR4), a comprehensive review of current knowledge about climate change, which will be published in 2007.

CRD Report

CRD Report is published every other month, highlighting recent achievements by staff members in Berkeley Lab's Computational Research Division. Distributed via email and posted on the Web at http://crd.lbl.gov/DOEresources, CRD Report may be freely distributed. CRD Report is edited by Jon Bashor, JBashor@lbl.gov or 510-486-5849.

Combustion Research Featured on PNAS Cover (continued from p.1)

"Although collaborations between computational scientists and experimentalists are becoming increasingly common, the results from this project clearly demonstrate how scientific computing is coming into its own as an essential component of scientific discovery," said Horst Simon, Associate Laboratory Director for Computing Sciences at Berkeley Lab. "The simulation is unprecedented in several aspects — the number of chemical species included, the number of chemical processes modeled, and the overall size of the flame. This is truly breakthrough computational science."



The article, written by John B. Bell, Marc S. Day, Ian G. Shepherd, Matthew R. Johnson, Robert K. Cheng, Joseph F. Grcar, Vincent E. Beckner and Michael J. Lijewski, describes the simulation of "a laboratory-scale turbulent rod-stabilized premixed methane V-flame. This simulation, which models a full laboratory-scale flame by using detailed chemistry and transport, encompasses a domain more than three orders of magnitude larger in volume than that of any previous efforts and represents a major increment in simulation complexity."

The LBNL combustion simulations use a different mathematical approach than has been typically used. Most other combustion simulations without turbulence models use equations that include sound waves, making them very computationally expensive. Because of this, such simulations often have been limited to only two dimensions, to scales less than a centimeter, or to just a few carbon species and reactions. By contrast, the LBNL researchers have modeled a three-dimensional flame about 12 cm high and consisting of 19 chemical species and 84 fundamental chemical reactions, producing results that could be compared directly with experimental diagnostics.

The LBNL group has developed an algorithmic approach that combines the "low Mach-number equations," which remove sound waves, with "adaptive mesh refinement" (AMR). The combined methodology strips away relatively unimportant aspects of the simulation and focus computing resources on the most important processes. Developed with the support of the Applied Mathematics Program of the DOE Office of Advanced Scientific Computing Research, the group's algorithms have slashed computational costs for combustion simulations by a factor of 10,000. Even so, the combustion simulation required substantial computing power — the simulation ran for about 1,000 hours on 256 processors of the IBM SP supercomputer at DOE's National Energy Research Scientific Computing Center.

The collaboration between computational and combustion scientists described in the National Academy Proceedings was supported by the Applied Partial Differential Equations Center (APDEC) of DOE's Scientific Discovery through Advanced Computation (SciDAC) program. The combustion experiments were supported by DOE's Office of Basic Energy Sciences in the Office of Science. The work also received support from Cristina Siegerist and Wes Bethel of LBNL's Visualization Group.

Researchers and institutions with a subscription to the Proceedings of the National Academy of Sciences can access the paper at <http://www.pnas.org/cgi/content/short/102/29/10006>.